Supporting information for the article “The ReaxFF Reactive Force Field for Solid Oxide Fuel Cell Systems with Application to Oxygen Ion Transport in Yttria-Stabilized Zirconia” by Adri C.T. van Duin, Boris V. Merinov, Seung Soon Jang, and William A. Goddard III

Reactive MD-force field: BaZrYOH fuel cells March 2007.

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 39       ! Number of general parameters
   50.0000 !Overcoordination parameter
    9.5469 !Overcoordination parameter
   26.5405 !Valency angle conjugation parameter
    3.0000 !Triple bond stabilisation parameter
    6.5000 !Triple bond stabilisation parameter
    0.0000 !C2-correction
    1.0588 !Undercoordination parameter
    9.0000 !Triple bond stabilisation parameter
   12.1176 !Undercoordination parameter
   13.3056 !Undercoordination parameter
    0.0000 !Triple bond stabilization energy
    0.0000 !Lower Taper-radius
   10.0000 !Upper Taper-radius
    2.8793 !Not used
   33.8667 !Valency undercoordination
    6.0891 !Valency angle/lone pair parameter
    1.0563 !Valency angle
    2.0384 !Valency angle parameter
    6.1431 !Not used
    6.9290 !Double bond/angle parameter
    0.3989 !Double bond/angle parameter: overcoord
    3.9954 !Double bond/angle parameter: overcoord
   -2.4837 !Not used
    5.7796 !Torsion/BO parameter
   10.0000 !Torsion overcoordination
    1.9487 !Torsion overcoordination
   -1.2327 !Conjugation 0 (not used)
    2.1645 !Conjugation
    1.5591 !vdWaals shielding
    0.0100 !Cutoff for bond order (*100)
    2.1365 !Valency angle conjugation parameter
    2.0000 !Overcoordination parameter
    3.0000 !Overcoordination parameter
    1.8512 !Valency/lone pair parameter
    0.5000 !Not used
   20.0000 !Not used
    5.0000 !Molecular energy (not used)
    0.0000 !Molecular energy (not used)
    2.6962 !Valency angle conjugation parameter
  8    ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
            alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
            cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
            ov/un;val1;n.u.;val3,vval4
C     1.3644   4.0000  12.0000   1.9803   0.1720   0.8712   1.2395   4.0000
      9.4734   2.1241   4.0000  31.8793  79.5548   5.7254   6.9235   0.0000
      1.2636   0.0000  -0.0537   5.7133  33.5629  11.9957   0.8563   0.0000
     -2.8983   4.7820   1.0564   4.0000   2.9663   0.0000   0.0000   0.0000
H     0.6853   1.0000   1.0080   1.3588   0.0622   0.7625  -0.1000   1.0000
      9.3992   5.0518   1.0000   0.0000 121.1250   3.8520   9.3303   1.0000
     -0.1000   0.0000  -0.1609   3.9714   3.2094   0.9031   1.0698   0.0000
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   -15.7683   3.3504   1.0338   1.0000   2.8793   0.0000   0.0000   0.0000
O    1.2891   2.0000  15.9990   1.9741   0.0880   0.8659   1.0323   6.0000
    10.2186   7.7719   4.0000  30.8697 116.0768   8.5000   6.9585   2.0000
     0.9456   4.1347  -1.3533  20.7724   3.5512   0.5074   0.9745   0.0000
    -3.6141   2.7025   1.0493   4.0000   2.9225   0.0000   0.0000   0.0000
N    1.2333   3.0000  14.0000   1.9324   0.1376   0.8596   1.1748   5.0000
    10.0667   7.8431   4.0000  32.2482 100.0000   6.8418   6.3404   2.0000
     1.0433  13.7673  -1.1806   2.1961   3.0696   2.7683   0.9745   0.0000
    -4.3875   2.6192   1.0183   4.0000   2.8793   0.0000   0.0000   0.0000
Zr   2.6383   4.0000  91.2240   2.2842   0.2481   0.5792  -1.0000   4.0000
    11.6632  48.5301   4.0000  -5.0000   0.0000  -1.5489   6.1282   0.0000
    -1.0000   0.0000 143.1770  48.2657   0.2144   0.0000   0.8563   0.0000
    -4.3695   3.3675   1.0338   8.0000   2.2632   0.0000   0.0000   0.0000
Y    2.7973   3.0000  88.9052   2.4630   0.2892   0.4474  -1.0000   3.0000
    11.9899  50.0000   3.0000  -5.0000   0.0000  -7.2157   7.8528   0.0000
    -1.0000   0.0000 143.1770 127.9235  78.0398   0.0000   0.8563   0.0000
    -2.5000   2.9867   1.0338   3.0000   2.5791   0.0000   0.0000   0.0000
Ba   2.5456   2.0000 137.3270   2.7000   0.2962   0.6301  -1.0000   2.0000
    10.3042  47.4978   2.0000  -5.0000   0.0000  -2.4182   5.5000   0.0000
    -1.0000   0.0000 143.1770 109.4891   9.4011   0.0147   0.8563   0.0000
    -7.5000   2.9867   1.0338   2.0000   2.5791   0.0000   0.0000   0.0000
X   -0.1000   2.0000   1.0080   2.0000   0.0000   1.0000  -0.1000   6.0000
    10.0000   2.5000   4.0000   0.0000   0.0000   8.5000   1.5000   0.0000
    -0.1000   0.0000  -2.3700   8.7410  13.3640   0.6690   0.9745   0.0000
   -11.0000   2.7466   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
22      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                       pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr
 1  1 139.8093 110.6913  77.2102   0.2737  -0.7584   1.0000  38.4226   0.3288
       0.1235  -0.2010   8.6973   1.0000  -0.1042   6.1688   1.0000   0.0000
 1  2 159.8520   0.0000   0.0000  -0.4646   0.0000   1.0000   6.0000   0.6170
      12.3878   1.0000   0.0000   1.0000  -0.0098   8.5954   0.0000   0.0000
 2  2 170.0433   0.0000   0.0000  -0.3573   0.0000   1.0000   6.0000   0.7489
       9.6471   1.0000   0.0000   1.0000  -0.0169   5.8818   0.0000   0.0000
 1  3 161.6647  58.4169 126.5609   0.2952  -0.1638   1.0000  12.1551   0.4055
       0.3211  -0.2388   7.5568   1.0000  -0.1729   4.9857   0.0000   0.0000
 3  3  87.8137 171.0665  40.0000   0.9810  -0.2106   1.0000  29.4721   1.0000
       0.8827  -0.1679   7.7980   1.0000  -0.1290   7.0000   1.0000   0.0000
 1  4 134.4562 139.7869  80.3761   0.0334  -0.1113   1.0000  27.0713   0.2076
       0.1315  -0.3049   7.0000   1.0000  -0.1355   5.2219   1.0000   0.0000
 3  4 130.8596 169.4551  40.0000   0.3837  -0.1639   1.0000  35.0000   0.2000
       1.0000  -0.3579   7.0004   1.0000  -0.1193   6.8773   1.0000   0.0000
 4  4 157.9384  82.5526 152.5336   0.4010  -0.1034   1.0000  12.4261   0.5828
       0.1578  -0.1509  11.9186   1.0000  -0.0861   5.4271   1.0000   0.0000
 2  3 198.1847   0.0000   0.0000  -0.4899   0.0000   1.0000   6.0000   0.3987
       2.4577   1.0000   0.0000   1.0000  -0.0549   5.6546   0.0000   0.0000
 2  4 231.8173   0.0000   0.0000  -0.3364   0.0000   1.0000   6.0000   0.4402
       8.8910   1.0000   0.0000   1.0000  -0.0327   6.5754   0.0000   0.0000
 5  5  74.5027   0.0000   0.0000  -0.2541  -0.2000   0.0000  16.0000   0.3564
       0.5882  -0.2000  15.0000   1.0000  -0.1315   6.4024   0.0000   0.0000
 3  5 112.4500   0.0000   0.0000   0.3505  -0.3000   1.0000  36.0000   0.4053
       0.1765  -0.2000  15.0000   1.0000  -0.1300  10.6008   1.0000   0.0000
 2  5  38.8626   0.0000   0.0000  -0.1577   0.0000   1.0000   6.0000   0.5000
      17.8821   1.0000   0.0000   1.0000  -0.2095   6.3931   0.0000   0.0000
 6  6  64.9243   0.0000   0.0000  -0.2933  -0.2000   0.0000  16.0000   0.3630
       1.3309  -0.2000  15.0000   1.0000  -0.0513   7.1116   0.0000   0.0000
 3  6 146.8558   0.0000   0.0000  -0.0215  -0.3000   1.0000  36.0000   0.8913
       0.0564  -0.2000  15.0000   1.0000  -0.1659   7.0537   1.0000   0.0000
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 2  6  38.8626   0.0000   0.0000  -0.1577   0.0000   1.0000   6.0000   0.2901
       17.8821   1.0000   0.0000   1.0000  -0.2095   6.3931   0.0000   0.0000
 5  6  63.5575   0.0000   0.0000  -0.1255  -0.2000   0.0000  16.0000   0.4238
        0.5959  -0.2000  15.0000   1.0000  -0.0923   7.4284   0.0000   0.0000
 3  7  29.1935   0.0000   0.0000  -0.1434  -0.3000   1.0000  36.0000   0.2069
        0.5062  -0.2000  15.0000   1.0000  -0.0559   7.0193   1.0000   0.0000
 2  7  38.8626   0.0000   0.0000  -0.1577   0.0000   1.0000   6.0000   0.2901
       17.8821   1.0000   0.0000   1.0000  -0.2095   6.3931   0.0000   0.0000
 5  7  87.4453   0.0000   0.0000   0.0004  -0.2000   0.0000  16.0000   0.2593
        1.0000  -0.2000  15.0000   1.0000  -0.0864   5.4765   0.0000   0.0000
 6  7  21.0000   0.0000   0.0000   0.0004  -0.2000   0.0000  16.0000   0.6594
        1.0000  -0.2000  15.0000   1.0000  -0.1155   9.0213   0.0000   0.0000
 7  7  30.1404   0.0000   0.0000   0.0004  -0.2000   0.0000  16.0000   0.4086
        1.0000  -0.2000  15.0000   1.0000  -0.0439   5.2951   0.0000   0.0000
15    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
 1  2   0.0431   1.7204  10.3632   1.0386  -1.0000  -1.0000
 2  3   0.0468   1.9998  10.2265   0.9368  -1.0000  -1.0000
 2  4   0.1059   1.8290   9.7818   0.9598  -1.0000  -1.0000
 1  3   0.1142   1.9602   9.4709   1.3065   1.1260   1.0865
 1  4   0.1445   1.8771  10.0000   1.7000   1.1885   1.1363
 3  4   0.1058   2.0043  10.1244   1.7000   1.1096   1.0206
 3  5   0.1473   1.7130  12.0284   1.9555  -1.0000  -1.0000
 3  6   0.1114   1.7581  13.0000   1.7808  -1.0000  -1.0000
 3  7   0.2824   1.7518  13.0000   2.1585  -1.0000  -1.0000
 5  7   0.2904   2.5610  12.9818   2.4596  -1.0000  -1.0000
 6  7   0.2079   2.1282  11.3529   2.4769  -1.0000  -1.0000
 5  6   0.2936   2.2035  12.2199   2.5822  -1.0000  -1.0000
 2  5   0.1000   1.7610  10.4809   0.1000  -1.0000  -1.0000
 2  6   0.1000   1.7610  10.4809   0.1000  -1.0000  -1.0000
 2  7   0.1000   1.7610  10.4809   0.1000  -1.0000  -1.0000
56    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
 1  1  1  75.8304  33.9168   0.8043   0.0000   0.1780  10.5736   1.0400
 1  1  2  69.6421   9.2578   3.6521   0.0000   0.0058   0.0000   1.0400
 2  1  2  75.4958  14.5436   2.7438   0.0000   0.0127   0.0000   1.0400
 1  2  2   0.0000   0.0000   6.0000   0.0000   0.0000   0.0000   1.0400
 1  2  1   0.0000   3.4110   7.7350   0.0000   0.0000   0.0000   1.0400
 2  2  2   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000   1.0400
 1  1  3  78.2305  16.3043   3.3209   0.0000   1.1127   0.0000   1.1880
 3  1  3  80.2229  45.0000   2.6995   0.0000   1.1127   0.0000   1.1880
 1  1  4  66.1305  41.9072   1.4346   0.0000   1.1127   0.0000   1.1880
 3  1  4  73.9544  45.0000   1.5778   0.0000   1.1127   0.0000   1.1880
 4  1  4  64.1581  45.0000   0.6370   0.0000   1.1127   0.0000   1.1880
 2  1  3  66.0941  11.3875   3.9388   0.0000   0.0755   0.0000   1.0500
 2  1  4  74.2929  10.7059   6.3074   0.0000   0.0755   0.0000   1.0500
 1  2  4   0.0000   0.0019   6.3000   0.0000   0.0000   0.0000   1.0400
 1  3  1  72.6402  38.4252   1.3200   0.0000   0.6142   0.0000   1.0783
 1  3  3  88.5142  45.0000   0.7808   0.0000   0.6142   0.0000   1.0783
 1  3  4  82.4890  43.2625   1.1759   0.0000   0.6142   0.0000   1.0783
 3  3  3  80.7324  35.1410   1.4999   0.0000   0.6142   0.0000   1.0783
 3  3  4  84.3637  25.1714   2.5361   0.0000   0.6142   0.0000   1.0783
 4  3  4  89.7071  45.0000   1.2301   0.0000   0.6142   0.0000   1.0783
 1  3  2  77.4332  39.5610   1.3429   0.0000   0.1218   0.0000   1.0500
 2  3  3  85.7907  10.5506   6.2301   0.0000   0.1218   0.0000   1.0500
 2  3  4  75.6201  45.0000   2.5874   0.0000   0.1218   0.0000   1.0500
 2  3  2  78.9033  33.3823   1.7364   0.0000   0.1218   0.0000   1.0500
 1  4  1  66.0330  22.0295   1.4442   0.0000   1.6777   0.0000   1.0500
 1  4  3 103.3204  33.0381   0.5787   0.0000   1.6777   0.0000   1.0500
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 1  4  4 104.1335   8.6043   1.6495   0.0000   1.6777   0.0000   1.0500
 3  4  3  74.1978  42.1786   1.7845 -18.0069   1.6777   0.0000   1.0500
 3  4  4  74.8600  43.7354   1.1572  -0.9193   1.6777   0.0000   1.0500
 4  4  4  75.0538  14.8267   5.2794   0.0000   1.6777   0.0000   1.0500
 1  4  2  69.1106  25.5067   1.1003   0.0000   0.0222   0.0000   1.0369
 2  4  3  81.3686  40.0712   2.2396   0.0000   0.0222   0.0000   1.0369
 2  4  4  83.0104  43.4766   1.5328   0.0000   0.0222   0.0000   1.0500
 2  4  2  70.8687  12.0168   5.0132   0.0000   0.0222   0.0000   1.1243
 1  2  3   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 1  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 1  2  5   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 3  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 4  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 2  2  3   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 2  2  4   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 3  2  3   0.0000   5.0000   3.0000   0.0000   0.0000   0.0000   1.0400
 2  3  5  42.5058  10.0776   5.0000   0.0000   0.9289   0.0000   1.1912
 2  3  6  50.0000   4.9111   1.0014   0.0000   1.0000   0.0000   1.1000
 2  3  7  90.0000   4.4647   1.6312   0.0000   1.0000   0.0000   1.1000
 3  5  3  55.8643  20.0000   0.3771   0.0000   0.1000   0.0000   1.4634
 3  6  3  50.0000  20.0000   4.0000   0.0000   1.8576   0.0000   2.8010
 3  7  3  90.0000   1.9850   5.0000   0.0000   0.2383   0.0000   1.2332
 5  3  5   5.9871   8.9966   0.2147   0.0000   2.7977   0.0000   3.0000
 5  3  6   8.1047   0.0887   0.1451   0.0000   0.1000   0.0000   2.8519
 5  3  7  62.7913   3.1555   2.9321   0.0000   1.8172   0.0000   1.4679
 6  3  6   3.0435   5.9522   9.0000   0.0000   1.6570   0.0000   1.1000
 6  3  7  79.3434   1.5639   1.7219   0.0000   1.3741   0.0000   2.3497
 7  3  7  54.7688   2.3715   3.0312   0.0000   1.6441   0.0000   1.4931
 3  3  5  80.0000  10.0000   1.2500   0.0000   0.5554   0.0000   1.2000
 3  3  6  80.0000  15.0000   1.2500   0.0000   0.5554   0.0000   1.2000
14    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 1  1  1  1   0.0000  38.9174   0.3649  -8.2931  -2.0127   0.0000   0.0000
 1  1  1  2   0.0000  49.1001   0.2713  -8.5284  -1.5309   0.0000   0.0000
 2  1  1  2   0.0000  34.0265   0.3804  -6.3917  -0.9965   0.0000   0.0000
 0  1  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  2  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  1  3  0   3.9830  13.0320   0.4739  -1.9813  -2.0000   0.0000   0.0000
 0  2  3  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  3  3  0   0.0318  23.1045   1.2614 -12.3670   0.0000   0.0000   0.0000
 0  1  4  0  -2.4242 128.1636   0.3739  -6.6098  -2.0000   0.0000   0.0000
 0  2  4  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  3  4  0   1.4816  55.6641   0.0004  -7.0465  -2.0000   0.0000   0.0000
 0  4  4  0  -0.3244  27.7086   0.0039  -2.8272  -2.0000   0.0000   0.0000
 0  1  1  0   0.0000   0.6675   0.0000  -8.2352   0.0000   0.0000   0.0000
 4  1  4  4  -5.5181   8.9706   0.0004  -6.1782  -2.0000   0.0000   0.0000
 4    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
 3  2  3   1.4000  -1.7731   1.4695   3.5257
 3  2  4   1.6337 -11.7496   1.4695   3.5257
 4  2  3   1.3999  -9.6921   1.4695   3.5257
 4  2  4   1.7514  -7.5768   1.4695   3.5257
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Tables of the energies used in Figures 2-7.

The periodic QM calculations were carried out using the SeqQuest code [1], which employs Gaussian basis functions rather than the plane wave basis often used in periodic systems. Nonlocal ECP or PP [2, 3] similar to those in Ref. [4] but for use in periodic systems were employed to replace the core electrons. These calculations used double zeta plus polarization contracted Gaussian functions [5] optimized for periodic calculations.

[1]. P.A. Schultz, unpublished [a description of the method is in P.J. Feibelman Phys. Rev. B 35, 2626 (1987).
[2]. C.F. Melius, W.A. Goddard III, Phys. Rev. A 10, 1528 (1974).
[3]. N. Troullier, J.L. Martins, Troullier, J.L. Martins, Phys. Rev B 43, 1993 (1991).
[4]. W.A. Goddard III, Phys. Rev. 174, 659 (1968).
[5]. P.A. Schultz, unpublished; see http://dft.sandia.gov/Quest.

Table 1. QM- and ReaxFF volume/energy data for Zr-fcc metal. All energies are relative to the Zr-fcc equilibrium volume.

Volume ($Å^3$)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
27.04	3	3.2
26.1	1.8	2
25.2	0.9	1
24.4	0.3	0.34
23.6	0	0
22.7	0.1	0.02
21.9	0.6	0.46
21.2	1.5	1.34
20.4	2.9	2.71
19.7	4.7	4.6
19	7.2	7.02

Table 2. QM- and ReaxFF volume/energy data for Zr-bcc metal. All energies are relative to the Zr-fcc ground state volume.

Volume ($Å^3$)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
28.8	8.9	8.26
27.7	6.1	6.36
26.5	4	4.66
25.4	2.6	3.16
24.3	1.9	2.06
23.3	1.8	1.46
22.3	2.3	1.36
21.3	3.2	1.86
20.3	4.6	3.26
19.4	6.5	5.46
18.5	8.7	8.76

Table 3. QM- and ReaxFF volume/energy data for Zr-a15 metal. All energies are relative to the Zr-fcc ground state volume.

Volume (Å^3)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
26.7	6.3	5.96
26	5.3	5.06
25.3	4.6	4.26
24.7	4	3.66
24	3.6	3.2
23.3	3.4	2.96
22.7	3.4064	2.95
22.1	3.7	3.19
21.4	4.2	3.72
20.8	5	4.56
19.7	7.5	7.36
18.5	11.4	11.76
17.4	16.7	18.16
16.4	23.9	26.96

Table 4. QM- and ReaxFF volume/energy data for Zr-simple cubic metal. All energies are relative to the Zr-fcc ground state volume.

Volume (Å^3)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
28.9	24.1	28.5
27.4	22.7	25.5
26	22.1	23.14
24.7	22.3	21.27
23.3	23.1	19.6
22.1	24.5	18.3
20.8	26.4	17.1
19.7	28.7	17.3

Table 5. QM- and ReaxFF volume/energy data for Y-fcc metal. All energies are relative to the Y-fcc ground state volume.

Volume (Å^3)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
48	15	15
41.2	6.1	6.8
37.8	2.6	3
35.6	1	1.1
34	0.2	0.24
32.6	0	0
31.3	0.2	0.3
30.3	0.7	0.8
29.3	1.4	1.9

Table 6. QM- and ReaxFF volume/energy data for Y-bcc metal. All energies are relative to the Y-fcc ground state volume.

Volume (Å^3)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
48.4	16.8	16.6
41.9	8.5	9.5
38.6	5.3	6.1
36.2	3.5	4
34.4	2.7	2.8
33	2.5	2.1

31.8	2.7	2.2
30.7	3.2	2.4
29.6	4	3
28.8	4.9	4
27.9	6	5.3
26	9.3	10
24.3	13.7	17.4

Table 7. QM- and ReaxFF volume/energy data for Y-simple cubic metal. All energies are relative to the Y-fcc ground state volume.

Volume ($Å^3$)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
54.3	32.1	17.3
45.5	23.2	14.3
40.4	19.6	17.8
37.4	18.2	20.8
35.1	17.8	23.3
33.2	18	26.8
31.7	18.7	30.3
30.4	19.6	33.3
29.3	20.8	36.3
28.3	22.1	40.3
26.3	25.7	49.3
24.7	30.1	62.3

Table 8. QM- and ReaxFF volume/heat of formation data for the bcc YZr alloy.

Volume ($Å^3$)	ΔH_f (QM) (kcal/mol)	ΔH_ϕ (ReaxFF) (kcal/mol)
33.608	22.1	17.5
29.805	13.4	8.9
28.25	11.7	6.9
27.4	11.4	6.1
26.6	11.6	5.7
25.55	12.7	5.9
24.1	15.8	7.8
21.55	26.7	18.6
19.85	38.9	34
18.55	51.9	52.3
17.55	87.4	85.7

Table 9. QM- and ReaxFF volume/heat of formation data for the fcc YZr_3 alloy.

Volume ($Å^3$)	ΔH_f (QM) (kcal/mol)	ΔH_ϕ (ReaxFF) (kcal/mol)
29.775	24.1	24
27.1	12.1	15.4
25.825	9.5	13.4
25.2	9.1	13.2
24.575	9.4	13.6
23.7	11.1	15.4
22.475	16.3	21
20.7	31.5	37.5
19.35	51.1	59.4
18.23	73.5	85.7

17.31	97	114.4

Table 10. QM- and ReaxFF volume/heat of formation data for the a15 YZr_3 alloy.

Volume (Å^3)	ΔH_f (QM) (kcal/mol)	ΔH_ϕ (ReaxFF) (kcal/mol)
34.3	67.5	60.9
31.95	58.1	39.15
30.65	56.6	38.9
29.5125	57.9	40.1
28.0375	63.8	45.9
25.925	82.2	67.9
22.6625	137.5	154.4
20.625	195.9	263.5
19.132	255.6	385.4
17.94	317.3	514.9

Table 11. QM- and ReaxFF volume/heat of formation data for the tetragonal YZr alloy.

Volume (Å^3)	ΔH_f (QM) (kcal/mol)	ΔH_ϕ (ReaxFF) (kcal/mol)
42.9	69.4	60
34	48.9	32.6
31.3	46	30.6
29.8	45.6	34.5
28.55	46	39.6
27.35	47	47.6

Table 12. QM- and ReaxFF volume/energy data for the monoclinic ZrO_2-phase. All energies are relative to the monoclinic ZrO_2 equilibrium volume.

Volume/ZrO_2 (Å^3)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
37.4555	0.5	0.74
36.757	0.1	0
36.556	0.04	0.05
36.33075	0	0.15
36.14775	0.01	0.23
35.9395	0.03	0.38
35.188	0.3	0.95
33.7975	1.6	2.9
31.328	7	8.7
29.968	11.8	13.75

Table 13. QM- and ReaxFF volume/energy data for the tetragonal ZrO_2-phase. All energies are relative to the monoclinic ZrO_2 equilibrium volume.

Volume/ZrO_2 (Å^3)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
37.3	2.9	3.3
36.1	1.6	1.3
35.4	1.3	2.3
35.3	1.24	2.8
35.1	1.2	3
34.9	1.21	3.1
34.7	1.21	3.2
34.1	1.3	3.6
32.9	2.7	5

31.7	5.2	8.6

Table 14. QM- and ReaxFF volume/energy data for the cubic ZrO_2-phase. All energies are relative to the monoclinic ZrO_2 equilibrium volume.

Volume/ZrO_2 (Å^3)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
37.9	9.9	7.5
35.6	5.1	3.8
34.7	4.1	1.84
34.2	3.85	1.75
33.9	3.8	1.8
33.6	3.83	2.1
33.2	4	2.6
32.6	4.7	3
32	5.7	4.5
31.5	7.1	5.5
30.5	10.4	8
29.7	14.4	10.5
29	19	13.1

Table 15. QM- and ReaxFF volume/energy data for the rutile ZrO_2-phase. All energies are relative to the monoclinic ZrO_2 equilibrium volume.

Volume/ZrO_2 (Å^3)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
47.4	19.7	23.7
42.1	7.4	7.2
40.7	5.83	5.2
40	5.46	4.4
39.55	5.4	4.2
39.15	5.45	4.31
38.6	5.7	4.9
37.7	6.7	6.3
36.25	9.8	10.3
35	14.2	13.5
33.95	19.5	15.8

Table 16. QM- and ReaxFF volume/energy data for the orthogonal ZrO_2-phase. All energies are relative to the monoclinic ZrO_2 equilibrium volume.

Volume/ZrO_2 (Å^3)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
36.6875	2	2
35.7	0.9	1.7
35.175	0.66	2
35	0.62	2.05
34.825	0.6	2.1
34.675	0.61	2.2
34.5	0.64	2.3
34.05	0.84	2.9
33.325	1.5	4.5
31.8	4.6	7.4
30.4875	9.3	10.1

Table 17. QM- and ReaxFF volume/energy data for the BaF_2 ZrO_2-phase. All energies are relative to the monoclinic ZrO_2 equilibrium volume.

Volume/ZrO_2 ($Å^3$)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
33.1	36.2	
32.6	36.02	
32.35	36	
32.1	36.02	
31.6	36.15	
31.15	36.4	
30.8	36.75	
30.25	37.45	
29.45	38.85	68
28.8	40.5	57
27.1		49
25.8		43
24.5		39
23.3		42
22.15		
21.055		

Table 18. QM- and ReaxFF volume/energy data for the cristobalite ZrO_2-phase. All energies are relative to the monoclinic ZrO_2 equilibrium volume.

Volume/ZrO_2 ($Å^3$)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
114.9	37.48	58.8
101.9	22.92	23.8
97.1	20.47	17.3
94.4	20.1	16.3
92.2	20.42	16.63
89.2	22.22	18.1
85.1	26.34	22.7
78.8	39.6	32.4
74.2	56.22	42.9
70.6	74.31	53.5
67.5	94.08	64.6

Table 19. QM- and ReaxFF volume/energy data for the Y_2O_3-phase (Y_2O_3 configuration). All energies are relative to the Y_2O_3 (Y_2O_3-configuration) equilibrium volume.

Volume/Y_2O_3 ($Å^3$)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
91.5125	18.4	7.5
84.5625	5.8	2
82.6625	3.3	1.19
81.01875	1.7	0.6
79.55	0.7	0.34
78.2125	0.15	0.16
76.96875	0	0
75.85	0.2	0.04
74.79375	0.7	0.31
73.8	1.4	0.81
72.875	2.4	1.5
72	3.5	2.3

70.0125	7.2	5.1
68.2875	11.5	8.5

Table 20. QM- and ReaxFF volume/energy data for the Y_2O_3-phase (conrundum configuration). All energies are relative to the Y_2O_3 (Y_2O_3-configuration) equilibrium volume.

Volume/Y_2O_3 (Å^3)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
90.5		10.04
82.27	11.8	6.28
78.25	7.4	6.54
76.18	6.5	6.8
74.97	6.3	7.04
73.82	6.5	7.34
72.23	7.3	7.94
69.87	9.9	9.14
65.17	18.6	14.14
62.45	30.9	18.14
59.48	45.9	27.94

Table 21. QM- and ReaxFF volume/energy data for the Y_2O_3-phase (trigonal configuration). All energies are relative to the Y_2O_3 (Y_2O_3-configuration) equilibrium volume.

Volume/Y_2O_3 (Å^3)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
90.3	43.3	41.6
76.9	13.1	23.9
73.1	9	19.6
71.2	8	18.1
70.1	7.9	17.5
69	8.1	17.1
67.6	8.8	17.1
65.4	11.2	18.2
61.9	18.8	25
59	29.2	36.8
56.6	41.4	51.7
54.6	54.5	67.9

Table 22. QM- and ReaxFF volume/energy data for a $Y_2Zr_6O_{15}$-phase ($Y_2O_3/(ZrO_2)_6$). All energies are relative to the equilibrium volume.

Volume/$Y_2Zr_6O_{15}$ (Å^3)	ΔE(QM) (kcal/mol)	ΔE(ReaxFF) (kcal/mol)
306.6	13.29	17.6
293.8	7.19	3.4
288.1	0	0.5
284.8	0.09	0
281.7	1.89	0.5
277.4	5.69	2.7
271.1	15.39	9.6
260.2	47.49	32.9
251.1	86.59	65.6
242.9	133.19	106.8
235.7	172.19	153.5

Table 23. QM- and ReaxFF ZrO_2-surface energies. All energies are relative to the monoclinic ZrO_2-phase at equilibrium volume.

Surface	ReaxFF (kcal/mol)	QM (kcal/mol)
101	6.26	4.6
001 oxygen terminated	9.51	6.88
001 Zr-terminated	21.76	26.4
100	9.23	8.23
110 oxygen terminated	9.72	8.16
110 Zr-terminated	20.56	25.8

The bgf-file for the final structure from the dynamics of the YSZ-14 structure at 1000K.

```
XTLGRF 200
DESCRP YSZ_RFF_prdc
RUTYPE NORMAL RUN
CRYSTX    20.86506   20.94317   20.89625   89.99634   90.00099   86.51411
FORMAT ATOM   (a6,1x,i5,1x,a5,1x,a3,1x,a1,1x,a5,3f10.5,1x,a5,i3,i2,1x,f8.5)
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0.00000
HETATM     2 O                    1.30648   1.72857   1.20190      O   4 0
0.00000
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HETATM     4 O                    6.37950   1.98115   3.18986      O   4 0
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HETATM     5 O                    1.14747   3.86591   3.19238      O   3 1
0.00000
HETATM     6 O                    1.43761   1.02137   3.88169      O   4 0
0.00000
HETATM     7 O                    4.66341   4.00982   3.79738      O   4 0
0.00000
HETATM     8 O                   -1.27359   4.26805   0.59511      O   4 0
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HETATM    18 O                    3.82023   9.19364   4.17622      O   4 0
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HETATM    19 O                    0.95846   8.47048   0.86287      O   4 0
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HETATM    20 O                    3.54016   6.67652   1.00139      O   4 0
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HETATM    21 Zr                  -0.35093   7.96915   2.45009      Zr  6 0
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HETATM    22 Zr                   2.07079   5.58845   2.61126      Zr  6 0
0.00000
HETATM    23 Zr                   2.69550   8.13070  -0.21055      Zr  6 0
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HETATM    24 Y                    0.20140  -0.92455   5.36119      Y   6 0
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HETATM   28 O                1.82467   7.10666   7.53106      O   3 1
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HETATM   29 O                1.00486   3.13585   8.96871      O   4 0
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HETATM   31 O                1.01586   3.29362   5.92366      O   4 0
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HETATM   34 Zr               2.91984   0.15511   7.52025      Zr  6 0
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HETATM   46 Zr               2.57928   7.76407   5.20180      Zr  6 0
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HETATM   47 Y               -0.11954  -0.60362   9.99229      Y   6 0
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HETATM   50 O                3.47710   1.96631  14.01881      O   4 0
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HETATM   52 O                1.00489   0.93066  14.03821      O   4 0
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HETATM    56 Zr                -0.01366   2.28460  12.79439      Zr  6 0
0.00000
HETATM    57 Zr                 2.66091   0.36441  12.69568      Zr  6 0
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HETATM    58 Y                  2.81857   3.27005  10.05853      Y   6 0
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HETATM    59 Zr                -0.42005   4.67875   9.43927      Zr  6 0
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HETATM    60 O                  0.44604   8.79505  15.07461      O   4 0
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HETATM    68 Zr                 0.54248   5.50110  12.52688      Zr  6 0
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HETATM    69 Zr                 2.25993   7.17891   9.62693      Zr  6 0
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HETATM    70 Y                  0.17891  -0.75457  15.17102      Y   6 0
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HETATM    99 O                4.54528  14.91657   3.29797      O   4 0
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HETATM   103 Zr               2.62670  10.97558   2.67348      Zr  6 0
0.00000
HETATM   104 Y                2.61667  13.19948  -0.26769      Y   6 0
0.00000
HETATM   105 Zr               0.16068  15.98351   0.13262      Zr  6 0
0.00000
HETATM   106 O                1.90186  17.19602   1.45132      O   4 0
0.00000
HETATM   107 O                2.93335  20.52848   0.55239      O   4 0
0.00000
HETATM   108 O                4.37242  17.95013   0.23363      O   4 0
0.00000
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HETATM  109 O                1.73615  19.27394   3.76816      O   3 1
0.00000
HETATM  110 O                4.12003  20.11011   3.05591      O   4 0
0.00000
HETATM  111 O                0.94398  19.85771   1.31654      O   4 0
0.00000
HETATM  112 O                6.18015  19.68602   1.48792      O   4 0
0.00000
HETATM  113 Zr               0.32656  18.15468   2.60098      Zr  6 0
0.00000
HETATM  114 Zr               2.64391  15.48179   2.39038      Zr  6 0
0.00000
HETATM  115 Zr               2.49840  18.63380  -0.17500      Zr  6 0
0.00000
HETATM  116 Y               -0.22810  10.45600   5.42200      Y   6 0
0.00000
HETATM  117 O                0.87982  11.62607   8.90396      O   4 0
0.00000
HETATM  118 O                3.79458  14.05841   7.17321      O   4 0
0.00000
HETATM  119 O                3.63058  12.24490   9.18067      O   4 0
0.00000
HETATM  120 O                0.82148  14.07890   9.26033      O   3 1
0.00000
HETATM  121 O                2.33162   9.24445   9.33399      O   4 0
0.00000
HETATM  122 O                3.57584  15.35841   9.43746      O   4 0
0.00000
HETATM  123 O                0.84952  14.95512   6.70214      O   4 0
0.00000
HETATM  124 O                4.47025  11.41549   7.31496      O   4 0
0.00000
HETATM  125 Zr               0.19773  13.12019   7.61173      Zr  6 0
0.00000
HETATM  126 Zr               2.66337  10.86191   7.91063      Zr  6 0
0.00000
HETATM  127 Y                2.90085  13.37415   5.22147      Y   6 0
0.00000
HETATM  128 Zr               0.07205  15.29107   4.81604      Zr  6 0
0.00000
HETATM  129 O                0.89164  18.05214   6.31665      O   4 0
0.00000
HETATM  130 O                4.83481  18.38763   4.93067      O   4 0
0.00000
HETATM  131 O                3.62044  16.40050   5.85533      O   4 0
0.00000
HETATM  132 O               -1.43732  18.59187   9.01596      O   3 1
0.00000
HETATM  133 O                6.59949  17.24959   6.29842      O   4 0
0.00000
HETATM  134 O                1.94841  20.21453   9.04346      O   4 0
0.00000
HETATM  135 O                3.64160  17.23605   3.44506      O   4 0
0.00000
HETATM  136 Zr              -0.38974  17.35526   7.63922      Zr  6 0
0.00000
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HETATM  137 Zr                2.68846  15.81974   7.76527      Zr  6 0
0.00000
HETATM  138 Zr                2.68233  17.97674   5.07785      Zr  6 0
0.00000
HETATM  139 Y                 0.37103   9.89478  10.31676      Y   6 0
0.00000
HETATM  140 O                 1.53054  12.22602  11.75982      O   4 0
0.00000
HETATM  141 O                 4.12611  14.77669  12.15341      O   4 0
0.00000
HETATM  142 O                 3.62973  12.18025  14.46645      O   4 0
0.00000
HETATM  143 O                 1.66402  15.67884  14.55270      O   3 1
0.00000
HETATM  144 O                 1.29672  12.20845  14.31199      O   4 0
0.00000
HETATM  145 O                 4.36438  14.88631  14.58672      O   4 0
0.00000
HETATM  146 O                 1.73062  14.47625  12.52007      O   4 0
0.00000
HETATM  147 O                 3.98365  12.35286  11.89458      O   4 0
0.00000
HETATM  148 Zr               -0.02815  13.22379  12.95453      Zr  6 0
0.00000
HETATM  149 Zr                2.63762  11.12411  12.92634      Zr  6 0
0.00000
HETATM  150 Y                 2.78475  13.77195  10.57098      Y   6 0
0.00000
HETATM  151 Zr                0.26718  15.62600  10.41205      Zr  6 0
0.00000
HETATM  152 O                 1.41558  16.23744  11.85101      O   4 0
0.00000
HETATM  153 O                 4.13154  20.07098  11.38588      O   4 0
0.00000
HETATM  154 O                 4.19584  17.43556  14.10998      O   4 0
0.00000
HETATM  155 O                 1.42444  18.55839  14.13910      O   3 1
0.00000
HETATM  156 O                 3.48550  19.77619  13.67820      O   4 0
0.00000
HETATM  157 O                 1.30390  18.96062  11.14206      O   4 0
0.00000
HETATM  158 O                 1.23431  16.92840   9.09663      O   4 0
0.00000
HETATM  159 Zr                0.27798  18.00685  12.55949      Zr  6 0
0.00000
HETATM  160 Zr                2.98507  16.15360  13.16096      Zr  6 0
0.00000
HETATM  161 Zr                2.91406  18.60606   9.90617      Zr  6 0
0.00000
HETATM  162 Y                 0.05974  10.95935  15.79573      Y   6 0
0.00000
HETATM  163 O                 1.23607  12.15510  17.34220      O   4 0
0.00000
HETATM  164 O                 6.28528  15.03383  16.97435      O   4 0
0.00000
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HETATM  165 O                3.84299  12.35958  19.10981      O   4 0
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HETATM  166 O                1.44703  14.62279  19.40342      O   3 1
0.00000
HETATM  167 O                1.20249  11.85086  19.39805      O   4 0
0.00000
HETATM  168 O                6.13551  14.80928  19.63269      O   4 0
0.00000
HETATM  169 O                0.46520  14.96530  17.18581      O   4 0
0.00000
HETATM  170 O                3.61248  14.54925  17.50084      O   4 0
0.00000
HETATM  171 Zr              -0.00617  13.27841  18.32530      Zr  6 0
0.00000
HETATM  172 Zr               2.39032  10.68850  18.35502      Zr  6 0
0.00000
HETATM  173 Y                2.47425  13.73906  15.57496      Y   6 0
0.00000
HETATM  174 Zr              -0.13073  16.16351  15.50556      Zr  6 0
0.00000
HETATM  175 O                1.34021  17.43321  16.78899      O   4 0
0.00000
HETATM  176 O                4.32475  19.28038  16.14300      O   4 0
0.00000
HETATM  177 O                4.15340  16.64595  18.88734      O   4 0
0.00000
HETATM  178 O                1.39283  17.46025  19.56514      O   3 1
0.00000
HETATM  179 O                3.88948  19.64618  18.83850      O   4 0
0.00000
HETATM  180 O                1.48845  19.72859  19.35014      O   4 0
0.00000
HETATM  181 O                3.82345  16.79666  16.58258      O   4 0
0.00000
HETATM  182 Zr              -0.08524  18.48993  18.39246      Zr  6 0
0.00000
HETATM  183 Zr               2.30270  16.17602  18.16397      Zr  6 0
0.00000
HETATM  184 Zr               2.81707  18.28149  15.44097      Zr  6 0
0.00000
HETATM  185 Y                5.03802  -0.17319  -0.53126      Y   6 0
0.00000
HETATM  186 O                6.03527   1.29848   1.05208      O   4 0
0.00000
HETATM  187 O                8.85573   6.64947   1.33907      O   4 0
0.00000
HETATM  188 O                8.99428   1.64152   3.04653      O   4 0
0.00000
HETATM  189 O                6.16810   7.17402   3.97598      O   3 1
0.00000
HETATM  190 O                6.53109   4.71352   1.30523      O   4 0
0.00000
HETATM  191 O                8.93658   4.48547   2.43921      O   4 0
0.00000
HETATM  192 O                4.72894   3.41749  -0.03188      O   4 0
0.00000
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HETATM  193 O                    8.66693   1.99924   1.24662      O   4 0
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HETATM  194 Zr                   5.26382   3.08577   1.91772      Zr  6 0
0.00000
HETATM  195 Zr                   7.45248   0.41102   2.01649      Zr  6 0
0.00000
HETATM  196 Y                    7.94000   3.65501  -0.28623      Y   6 0
0.00000
HETATM  197 Zr                   4.91735   5.54173  -0.33288      Zr  6 0
0.00000
HETATM  198 O                    5.86861   7.11202   1.47626      O   4 0
0.00000
HETATM  199 O                    8.65463   9.53075   1.23453      O   4 0
0.00000
HETATM  200 O                    7.31925   5.44444   4.68834      O   4 0
0.00000
HETATM  201 O                    6.99651   9.51777   4.54351      O   3 1
0.00000
HETATM  202 O                    9.44586   9.75544   3.70757      O   4 0
0.00000
HETATM  203 O                    6.25349   9.50288   1.87907      O   4 0
0.00000
HETATM  204 O                    8.93512   7.16804   3.81165      O   4 0
0.00000
HETATM  205 Zr                   4.58473   8.17367   2.46193      Zr  6 0
0.00000
HETATM  206 Zr                   7.43700   5.87807   2.62455      Zr  6 0
0.00000
HETATM  207 Zr                   7.30749   8.31242   0.32766      Zr  6 0
0.00000
HETATM  208 Y                    5.44895   0.17649   4.59295      Y   6 0
0.00000
HETATM  209 O                    6.90328   2.32877   6.77943      O   4 0
0.00000
HETATM  210 O                   11.61639   5.69416   5.66853      O   4 0
0.00000
HETATM  211 O                    9.46381   1.11043   8.93945      O   4 0
0.00000
HETATM  212 O                    4.41455   4.31246   8.73753      O   3 1
0.00000
HETATM  213 O                    6.43454   1.57126   8.85819      O   4 0
0.00000
HETATM  214 O                    8.49791   4.07543   8.33742      O   4 0
0.00000
HETATM  215 O                    5.95353   4.42622   6.60005      O   4 0
0.00000
HETATM  216 O                    9.28914   1.61775   6.28488      O   4 0
0.00000
HETATM  217 Zr                   5.09009   2.71678   7.53639      Zr  6 0
0.00000
HETATM  218 Zr                   7.78583   0.55963   7.54719      Zr  6 0
0.00000
HETATM  219 Y                    7.93467   2.63759   4.76004      Y   6 0
0.00000
HETATM  220 Zr                   5.23996   5.57179   4.87962      Zr  6 0
0.00000
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HETATM  221 O                9.36159   4.18416   5.53455      O   4 0
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HETATM  222 O                8.86683   9.61724   9.53077      O   4 0
0.00000
HETATM  223 O               11.67795   7.19364   9.59019      O   4 0
0.00000
HETATM  224 O                6.32672   7.41315   6.89605      O   3 1
0.00000
HETATM  225 O                7.04197   6.00655   8.74951      O   4 0
0.00000
HETATM  226 O                8.13403   9.27858   6.77389      O   4 0
0.00000
HETATM  227 O                9.21715   6.74449   6.77923      O   4 0
0.00000
HETATM  228 Zr               4.97312   6.22476   7.93528      Zr  6 0
0.00000
HETATM  229 Zr               7.98781   5.21304   6.81482      Zr  6 0
0.00000
HETATM  230 Zr               7.76427   7.76123   5.33841      Zr  6 0
0.00000
HETATM  231 Y                5.82194  -0.11023  10.30661      Y   6 0
0.00000
HETATM  232 O                6.35129   1.60051  11.90951      O   4 0
0.00000
HETATM  233 O                8.40845   6.29938  11.41242      O   4 0
0.00000
HETATM  234 O                8.73181   2.97578  14.17163      O   4 0
0.00000
HETATM  235 O                6.39478   5.89089  14.24239      O   3 1
0.00000
HETATM  236 O                6.20709   1.69646  14.15497      O   4 0
0.00000
HETATM  237 O               10.88812   4.76489  14.69600      O   4 0
0.00000
HETATM  238 O                5.86174   4.42246  11.89316      O   4 0
0.00000
HETATM  239 O                8.78402   3.16904  11.74301      O   4 0
0.00000
HETATM  240 Zr               4.94879   2.68503  12.94495      Zr  6 0
0.00000
HETATM  241 Zr               8.05487   1.43812  12.93371      Zr  6 0
0.00000
HETATM  242 Y                7.61384   4.39677  10.38174      Y   6 0
0.00000
HETATM  243 Zr               4.79229   5.92486  12.84031      Zr  6 0
0.00000
HETATM  244 O                5.80911   7.45704  11.86085      O   4 0
0.00000
HETATM  245 O                8.49248   9.52159  14.10559      O   4 0
0.00000
HETATM  246 O                9.08487   6.94845  14.31509      O   4 0
0.00000
HETATM  247 O               10.29972   8.76629  15.77770      O   3 1
0.00000
HETATM  248 O                6.44270   8.12133  15.01547      O   4 0
0.00000
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HETATM  249 O                    6.43643   7.35420  17.05010      O   4 0
0.00000
HETATM  250 O                    9.61710   8.46815  11.93955      O   4 0
0.00000
HETATM  251 Zr                   2.58708   7.94073  12.97652      Zr  6 0
0.00000
HETATM  252 Zr                   7.56708   7.61955  12.96923      Zr  6 0
0.00000
HETATM  253 Zr                   7.89173   8.01058   8.38918      Zr  6 0
0.00000
HETATM  254 Y                    5.64662  -0.04173  15.52642      Y   6 0
0.00000
HETATM  255 O                    4.45780   1.50966  17.60480      O   4 0
0.00000
HETATM  256 O                    9.28470   4.92602  16.94176      O   4 0
0.00000
HETATM  257 O                    8.29309   2.78977  16.97216      O   4 0
0.00000
HETATM  258 O                    6.60332   5.26777  19.41697      O   3 1
0.00000
HETATM  259 O                    6.77367   2.33459  19.25730      O   4 0
0.00000
HETATM  260 O                    9.25332   5.06223  19.19398      O   4 0
0.00000
HETATM  261 O                    6.32516   7.87625  19.55392      O   4 0
0.00000
HETATM  262 O                    9.68921   2.00217  19.30767      O   4 0
0.00000
HETATM  263 Zr                   5.05944   3.20204  18.57056      Zr  6 0
0.00000
HETATM  264 Zr                   8.02402   1.11956  18.31831      Zr  6 0
0.00000
HETATM  265 Y                    7.69213   4.31125  15.58332      Y   6 0
0.00000
HETATM  266 Zr                   5.17840   6.24326  16.00303      Zr  6 0
0.00000
HETATM  267 O                    5.62843   4.41900  16.90943      O   4 0
0.00000
HETATM  268 O                    9.41713  10.16597  18.05163      O   4 0
0.00000
HETATM  269 O                    9.03275   7.70359  19.92545      O   4 0
0.00000
HETATM  270 O                    4.04197   9.73433  19.81719      O   3 1
0.00000
HETATM  271 O                    7.07036  10.03831  20.06117      O   4 0
0.00000
HETATM  272 O                    6.87570   9.68183  17.12069      O   4 0
0.00000
HETATM  273 O                    9.13621   7.23737  17.30466      O   4 0
0.00000
HETATM  274 Zr                   5.17772   8.78353  18.32282      Zr  6 0
0.00000
HETATM  275 Zr                   7.76859   6.55539  18.66485      Zr  6 0
0.00000
HETATM  276 Zr                   8.12900   8.29679  15.95925      Zr  6 0
0.00000
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HETATM  277 Y                5.36307  10.94549   0.19541      Y   6 0
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HETATM  278 O                6.56333  12.07390   4.07699      O   4 0
0.00000
HETATM  279 O                8.78759  14.59285   2.29787      O   4 0
0.00000
HETATM  280 O                9.02776  12.14293   3.85063      O   4 0
0.00000
HETATM  281 O                6.72098  14.92891   3.98603      O   3 1
0.00000
HETATM  282 O               12.09454  12.49689   4.07246      O   4 0
0.00000
HETATM  283 O                9.94831  14.42904   4.91613      O   4 0
0.00000
HETATM  284 O                6.16876  14.57237   1.11663      O   4 0
0.00000
HETATM  285 O                7.21780  12.20894   1.77583      O   4 0
0.00000
HETATM  286 Zr               5.45771  13.25263   2.73190      Zr  6 0
0.00000
HETATM  287 Zr               7.79916  10.61519   3.03861      Zr  6 0
0.00000
HETATM  288 Y                8.09171  13.53527   0.41168      Y   6 0
0.00000
HETATM  289 Zr               5.29428  16.03602  -0.14550      Zr  6 0
0.00000
HETATM  290 O                6.38027  17.21529   1.18404      O   4 0
0.00000
HETATM  291 O                8.89195  19.82207   1.41885      O   4 0
0.00000
HETATM  292 O                8.81765  16.90122   3.81486      O   4 0
0.00000
HETATM  293 O                6.34596  17.75822   3.88227      O   3 1
0.00000
HETATM  294 O                9.82792  18.98928   4.45909      O   4 0
0.00000
HETATM  295 O                7.43562  20.22685   3.83494      O   4 0
0.00000
HETATM  296 O                9.46926  18.38499  -0.85049      O   4 0
0.00000
HETATM  297 Zr               4.81258  18.36161   2.40386      Zr  6 0
0.00000
HETATM  298 Zr               7.65141  16.25348   2.51440      Zr  6 0
0.00000
HETATM  299 Zr               7.67540  18.66561   0.27764      Zr  6 0
0.00000
HETATM  300 Y                5.24637   9.72051   5.80312      Y   6 0
0.00000
HETATM  301 O                6.96515  12.14613   6.82885      O   4 0
0.00000
HETATM  302 O                8.66909  14.25949   7.39181      O   4 0
0.00000
HETATM  303 O                9.20259  12.41618   9.28203      O   4 0
0.00000
HETATM  304 O                6.12105  17.24498   8.77573      O   3 1
0.00000
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HETATM  305 O                6.55832  11.99763   9.45809      O   4 0
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HETATM  306 O               10.63139  14.66905   9.53200      O   4 0
0.00000
HETATM  307 O                6.04681  14.71596   9.34235      O   4 0
0.00000
HETATM  308 O                9.76487  11.65397   7.17611      O   4 0
0.00000
HETATM  309 Zr               5.28818  13.07203   8.04270      Zr  6 0
0.00000
HETATM  310 Zr               7.95334  11.08338   8.29748      Zr  6 0
0.00000
HETATM  311 Y                7.88947  13.63390   5.27203      Y   6 0
0.00000
HETATM  312 Zr               5.47968  16.20437   4.85324      Zr  6 0
0.00000
HETATM  313 O                6.20934  14.76692   6.54400      O   4 0
0.00000
HETATM  314 O                6.43975  20.42391   6.51859      O   4 0
0.00000
HETATM  315 O                8.46488  16.36210   9.22087      O   4 0
0.00000
HETATM  316 O                7.48743  19.86605   8.76429      O   3 1
0.00000
HETATM  317 O                8.80871  19.74421   6.40393      O   4 0
0.00000
HETATM  318 O                3.71423  17.48251   8.39529      O   4 0
0.00000
HETATM  319 O                9.11919  17.21177   6.63130      O   4 0
0.00000
HETATM  320 Zr               5.27025  18.66932   7.01799      Zr  6 0
0.00000
HETATM  321 Zr               7.41479  15.91551   7.73506      Zr  6 0
0.00000
HETATM  322 Zr               7.87193  18.53390   5.03357      Zr  6 0
0.00000
HETATM  323 Y                5.23624   9.25260  10.51714      Y   6 0
0.00000
HETATM  324 O                7.01208   9.57198  11.85776      O   4 0
0.00000
HETATM  325 O                7.00394  12.78550  12.53628      O   4 0
0.00000
HETATM  326 O                9.05194  11.98930  14.44808      O   4 0
0.00000
HETATM  327 O                6.57899  15.00160  14.23307      O   3 1
0.00000
HETATM  328 O                5.98712  11.57797  13.82307      O   4 0
0.00000
HETATM  329 O                9.08817  14.56672  14.16600      O   4 0
0.00000
HETATM  330 O                6.94923  15.51982  11.71975      O   4 0
0.00000
HETATM  331 O                9.51150  11.57005  12.02614      O   4 0
0.00000
HETATM  332 Zr               5.21349  13.35665  13.32622      Zr  6 0
0.00000
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HETATM  333 Zr                7.86507  10.98492  13.01692      Zr  6 0
0.00000
HETATM  334 Y                 7.63588  13.57695  10.56924      Y   6 0
0.00000
HETATM  335 Zr                5.36971  16.31446  10.49576      Zr  6 0
0.00000
HETATM  336 O                 6.06108  18.28949  11.00206      O   4 0
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HETATM  337 O                 8.37371  20.69666  11.65974      O   4 0
0.00000
HETATM  338 O                 6.72946  17.44926  13.55142      O   4 0
0.00000
HETATM  339 O                 3.69542  17.22282  11.51443      O   3 1
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HETATM  340 O                 9.09177  20.88226  13.78383      O   4 0
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HETATM  341 O                 6.48102  19.79638  13.43754      O   4 0
0.00000
HETATM  342 O                 9.08731  17.77787  11.85427      O   4 0
0.00000
HETATM  343 Zr                4.98479  18.64437  12.79914      Zr  6 0
0.00000
HETATM  344 Zr                8.22974  16.12462  13.14193      Zr  6 0
0.00000
HETATM  345 Zr                7.77160  18.18913   9.77263      Zr  6 0
0.00000
HETATM  346 Y                 5.28472  10.04571  15.37349      Y   6 0
0.00000
HETATM  347 O                 6.52533  12.45802  16.92858      O   4 0
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HETATM  348 O                10.67184  15.25181  17.06845      O   4 0
0.00000
HETATM  349 O                 9.16235  12.50141  19.73153      O   4 0
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HETATM  350 O                 6.81280  17.80500  19.21640      O   3 1
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HETATM  351 O                 6.29979  12.26008  19.45698      O   4 0
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HETATM  352 O                 8.84836  14.98200  19.67528      O   4 0
0.00000
HETATM  353 O                 8.95992  17.05901  21.94651      O   4 0
0.00000
HETATM  354 O                 8.72612  12.99786  17.60137      O   4 0
0.00000
HETATM  355 Zr                5.27678  13.47323  18.20547      Zr  6 0
0.00000
HETATM  356 Zr                7.85051  11.33029  18.37645      Zr  6 0
0.00000
HETATM  357 Y                 7.78284  13.80158  15.79212      Y   6 0
0.00000
HETATM  358 Zr                5.49594  16.42141  15.37155      Zr  6 0
0.00000
HETATM  359 O                 8.27175  15.90357  16.19404      O   4 0
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HETATM  360 O                 7.23257  20.75484  16.92627      O   4 0
0.00000
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0.00000
HETATM  363 O                9.30876  20.62618  18.92866      O   4 0
0.00000
HETATM  364 O                6.69655  17.55535  16.67632      O   4 0
0.00000
HETATM  365 O                9.80892  19.41159  16.76942      O   4 0
0.00000
HETATM  366 Zr               4.87465  18.17492  17.97717      Zr  6 0
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HETATM  367 Zr               7.52547  16.11795  18.31353      Zr  6 0
0.00000
HETATM  368 Zr               7.98628  19.02354  17.98573      Zr  6 0
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HETATM  369 Y               10.63123   0.37701  -0.14090      Y   6 0
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HETATM  370 O               11.82045   1.85926   1.08307      O   4 0
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HETATM  371 O               14.12807   4.86049   1.41510      O   4 0
0.00000
HETATM  372 O               14.15092   2.53067   3.75870      O   4 0
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HETATM  373 O               11.50831   4.62060   2.85977      O   3 1
0.00000
HETATM  374 O               11.26170   1.75013   3.37277      O   4 0
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HETATM  375 O               13.85825   6.08222   4.47175      O   4 0
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HETATM  376 O               10.66671   4.18738   0.39133      O   4 0
0.00000
HETATM  377 O               14.64274   1.78827   1.38490      O   4 0
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HETATM  378 Zr              10.33625   2.95820   1.98990      Zr  6 0
0.00000
HETATM  379 Zr              13.28613   1.00932   2.64296      Zr  6 0
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HETATM  380 Y               12.76418   3.85876  -0.19617      Y   6 0
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HETATM  381 Zr              10.14281   6.17069  -0.21001      Zr  6 0
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HETATM  382 O               11.59947   6.76042   1.07601      O   4 0
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HETATM  383 O               14.33920   9.67519   1.96229      O   4 0
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HETATM  384 O               14.94056   8.31152   4.52751      O   4 0
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HETATM  385 O               11.42318   7.29212   3.61817      O   3 1
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HETATM  386 O               12.23545   9.61928   4.47192      O   4 0
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HETATM  387 O               11.83303   9.25476   1.67245      O   4 0
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HETATM  388 O               14.46964   7.34335   1.85237      O   4 0
0.00000
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HETATM  390 Zr                  13.02019   5.98365   2.50542      Zr  6 0
0.00000
HETATM  391 Zr                  13.21779   8.57339   0.36114      Zr  6 0
0.00000
HETATM  392 Y                   10.56227   0.26884   4.77557      Y   6 0
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HETATM  393 O                   12.05652   2.16637   6.92213      O   4 0
0.00000
HETATM  394 O                   14.76139   3.97847   6.46112      O   4 0
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HETATM  396 O                   10.98247   4.67030  11.39220      O   3 1
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HETATM  397 O                   11.54051   1.57151   9.03746      O   4 0
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HETATM  398 O                   14.84648   4.06520   8.84323      O   4 0
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HETATM  399 O                    9.47814   6.99312   9.15920      O   4 0
0.00000
HETATM  400 O                   14.54964   1.22376   6.63776      O   4 0
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HETATM  401 Zr                  10.28722   2.77515   7.73111      Zr  6 0
0.00000
HETATM  402 Zr                  12.76563   0.49793   7.78180      Zr  6 0
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HETATM  403 Y                   12.76829   3.83715   5.34860      Y   6 0
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HETATM  404 Zr                  10.07859   5.59064   4.15047      Zr  6 0
0.00000
HETATM  405 O                   11.60660   8.45671   6.85609      O   4 0
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HETATM  406 O                   14.12760  10.11271   7.23877      O   4 0
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HETATM  407 O                   14.05323   6.16163   9.26626      O   4 0
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HETATM  408 O                   11.78172   7.32406  12.55701      O   3 1
0.00000
HETATM  409 O                   15.26364   8.78705   9.40276      O   4 0
0.00000
HETATM  410 O                   13.14395   6.72203   7.06689      O   4 0
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HETATM  411 O                   15.22432   7.71141   7.17488      O   4 0
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HETATM  412 Zr                  11.04034   6.45472   7.73797      Zr  6 0
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HETATM  413 Zr                  15.25558   5.54352   7.53579      Zr  6 0
0.00000
HETATM  414 Zr                  12.87919   7.70669   5.15347      Zr  6 0
0.00000
HETATM  415 Y                   10.50114   0.10472  10.59504      Y   6 0
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HETATM  416 O                   11.52088   2.00047  12.32217      O   4 0
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HETATM  417 O                14.31585   5.56169  11.74812      O   4 0
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HETATM  418 O                15.00771   2.61092  14.08466      O   4 0
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HETATM  419 O                11.95527   7.59527  14.96405      O   3 1
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HETATM  420 O                11.96118   2.60058  14.09106      O   4 0
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HETATM  421 O                14.10008   5.51766  14.23580      O   4 0
0.00000
HETATM  422 O                11.38402   4.47363   8.15978      O   4 0
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HETATM  423 O                13.83675   3.03126  11.88011      O   4 0
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HETATM  424 Zr               10.43450   3.56247  13.02556      Zr  6 0
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HETATM  425 Zr               13.36931   1.55574  13.16624      Zr  6 0
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HETATM  426 Y                12.96639   4.24977  10.15318      Y   6 0
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HETATM  427 Zr               10.32722   6.71978  11.10448      Zr  6 0
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HETATM  428 O                14.29046   8.36716  14.88389      O   4 0
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HETATM  429 O                14.30882  10.62518  12.74093      O   4 0
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HETATM  430 O                16.68115   9.83554  14.82129      O   4 0
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HETATM  431 O                12.34824  10.41063  15.17878      O   3 1
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HETATM  432 O                11.68473  10.20280  12.92314      O   4 0
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HETATM  433 O                12.64336  10.13689   9.34347      O   4 0
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HETATM  434 O                14.35947   8.25582  11.76107      O   4 0
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HETATM  435 Zr               10.55336   8.78996  13.85668      Zr  6 0
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HETATM  436 Zr               13.51091   7.13514  13.13737      Zr  6 0
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HETATM  437 Zr               13.35628   8.25978   8.43666      Zr  6 0
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HETATM  438 Y                10.47805   0.16563  15.44334      Y   6 0
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HETATM  439 O                 9.77522   1.83575  16.96426      O   4 0
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HETATM  440 O                14.74813   5.03522  17.00185      O   4 0
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HETATM  441 O                14.84195   1.74884  19.09912      O   4 0
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HETATM  442 O                12.17487   5.92700  20.04481      O   3 1
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HETATM  443 O                11.92094   2.57344  18.92440      O   4 0
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HETATM  444 O                14.57294   4.72733  19.65426      O   4 0
0.00000
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HETATM   445 O                11.91689   4.72381  17.60249      O   4 0
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HETATM   447 Zr               10.29059   3.55842  17.93890      Zr  6 0
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HETATM   448 Zr               13.11501   1.20224  18.19577      Zr  6 0
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HETATM   449 Y                12.99862   4.18358  15.59651      Y   6 0
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HETATM   450 Zr               10.50881   6.37588  15.75562      Zr  6 0
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HETATM   451 O                12.00150   7.48110  17.62610      O   4 0
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HETATM   452 O                14.44431  10.34012  17.29183      O   4 0
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HETATM   453 O                14.28688   7.48413  20.03098      O   4 0
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HETATM   454 O                11.41982   9.04743  20.17591      O   3 1
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HETATM   455 O                13.90897  10.05956  19.70481      O   4 0
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HETATM   456 O                11.77859  10.04863  17.75226      O   4 0
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HETATM   457 O                14.51433   7.59714  17.24054      O   4 0
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HETATM   458 Zr               10.56900   8.43106  18.47186      Zr  6 0
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HETATM   459 Zr               13.31143   6.11759  18.41842      Zr  6 0
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HETATM   460 Zr               13.00618   8.77815  16.44282      Zr  6 0
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HETATM   461 Y                10.49664  10.92218  -0.01699      Y   6 0
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HETATM   462 O                10.99850  12.06055   1.89091      O   4 0
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HETATM   463 O                14.44354  15.13776   1.96417      O   4 0
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HETATM   464 O                14.59230  11.75737   3.89547      O   4 0
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HETATM   465 O                14.93836  14.76970   4.24653      O   3 1
0.00000
HETATM   466 O                12.06046  15.70742   4.32807      O   4 0
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HETATM   467 O                17.29110  16.22889   4.10450      O   4 0
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HETATM   468 O                11.74615  14.85654   2.09658      O   4 0
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HETATM   469 O                14.11143  12.30621   1.72092      O   4 0
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HETATM   470 Zr               10.46912  13.45829   3.09290      Zr  6 0
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HETATM   471 Zr               12.72484  11.05179   2.79011      Zr  6 0
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HETATM   472 Y                13.08108  14.47784   0.28600      Y   6 0
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HETATM  473 Zr                10.16139  16.49296  -0.69781      Zr  6 0
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HETATM  474 O                 11.58561  17.17911   1.00348      O   4 0
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HETATM  475 O                 14.26042  20.01509   1.20163      O   4 0
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HETATM  476 O                 14.11769  17.71478   3.75738      O   4 0
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HETATM  477 O                 12.48275  20.60538   4.11287      O   3 1
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HETATM  478 O                 14.80594  20.77098   2.99145      O   4 0
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HETATM  479 O                 11.17894  19.80686   1.40088      O   4 0
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HETATM  480 O                 14.20794  17.38786   1.18025      O   4 0
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HETATM  481 Zr                 9.92997  18.37610   2.33049      Zr  6 0
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HETATM  482 Zr                13.00486  16.39050   2.69183      Zr  6 0
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HETATM  483 Zr                12.80289  18.72616   0.47142      Zr  6 0
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HETATM  484 Y                 10.34334   9.84235   5.76346      Y   6 0
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HETATM  485 O                 11.87192  12.65633   6.83354      O   4 0
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HETATM  486 O                 14.09347  17.03979   8.87481      O   4 0
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HETATM  487 O                 15.00772  12.05139   9.21484      O   4 0
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HETATM  488 O                 11.72767  16.91469   9.27780      O   3 1
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HETATM  489 O                 12.33002  13.04517   9.35351      O   4 0
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HETATM  490 O                 16.75590  17.87542   8.89252      O   4 0
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HETATM  491 O                 11.10245  15.13533   6.82666      O   4 0
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HETATM  492 O                 14.46172  12.34735   6.57956      O   4 0
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HETATM  493 Zr                10.43245  13.46798   7.93277      Zr  6 0
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HETATM  494 Zr                13.23212  11.71792   8.26143      Zr  6 0
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HETATM  495 Y                 13.11924  13.86610   5.36856      Y   6 0
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HETATM  496 Zr                10.46593  16.29130   5.21609      Zr  6 0
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HETATM  497 O                 11.70824  17.70026   6.59540      O   4 0
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HETATM  498 O                 14.03328  17.19996   6.21663      O   4 0
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HETATM  499 O                 13.89865  19.83321   6.27025      O   4 0
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0.00000
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HETATM  501 O                12.26594  19.64980   8.60948      O   4 0
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HETATM  502 O                11.36021  20.41125   6.88868      O   4 0
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HETATM  503 O                11.17801  17.87466   3.84157      O   4 0
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HETATM  504 Zr               10.27632  18.71161   7.59032      Zr  6 0
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HETATM  505 Zr               12.65625  16.30055   7.48408      Zr  6 0
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HETATM  506 Zr               12.82336  18.66952   5.03322      Zr  6 0
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HETATM  507 Y                10.74928   9.96977  10.67407      Y   6 0
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HETATM  508 O                11.96764  13.03020  12.33773      O   4 0
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HETATM  509 O                14.71377  15.01477  11.36185      O   4 0
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HETATM  510 O                14.73867  15.49497  14.59681      O   4 0
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HETATM  511 O                11.23133  16.78386  14.40037      O   3 1
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HETATM  512 O                11.79222  13.24635  14.54430      O   4 0
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HETATM  513 O                17.22883  15.74720  14.04108      O   4 0
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HETATM  514 O                 9.43859  14.56146  11.73229      O   4 0
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HETATM  515 O                14.55378  12.91281  14.01090      O   4 0
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HETATM  516 Zr               10.15538  13.14660  13.18143      Zr  6 0
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HETATM  517 Zr               12.85026  11.67441  13.66451      Zr  6 0
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HETATM  518 Y                12.72208  14.57929  10.82119      Y   6 0
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HETATM  519 Zr               10.20631  16.30667  10.73021      Zr  6 0
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HETATM  520 O                11.93466  16.51092  11.81369      O   4 0
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HETATM  521 O                 9.34084  17.82607  14.28491      O   4 0
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HETATM  522 O                14.09030  18.05417  14.26144      O   4 0
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HETATM  523 O                12.17182  19.73206  14.51341      O   3 1
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HETATM  524 O                11.79056  19.30380  11.54822      O   4 0
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HETATM  525 O                14.26454  20.68757  12.38146      O   4 0
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HETATM  526 O                14.54440  18.03053  11.59880      O   4 0
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HETATM  527 Zr                8.20690  19.07027  12.92754      Zr  6 0
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HETATM  528 Zr               12.25266  18.13256  13.21298      Zr  6 0
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HETATM  529 Zr                12.99688  18.39390  10.05818      Zr  6 0
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HETATM  530 Y                 10.38943  11.00983  16.08164      Y   6 0
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HETATM  531 O                 11.68475  12.62006  17.27266      O   4 0
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HETATM  532 O                 13.80233  15.49076  17.13015      O   4 0
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HETATM  533 O                 14.08110  13.16473  19.64862      O   4 0
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HETATM  534 O                 12.07191  17.49756  19.75033      O   3 1
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HETATM  535 O                 11.71438  12.32471  19.69746      O   4 0
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HETATM  536 O                 14.45932  15.83048  19.67691      O   4 0
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HETATM  537 O                 11.28572  14.94746  19.86183      O   4 0
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HETATM  538 O                 14.45812  13.03263  17.17302      O   4 0
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HETATM  539 Zr                10.54009  13.76467  18.36542      Zr  6 0
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HETATM  540 Zr                13.20703  11.84495  18.33855      Zr  6 0
0.00000
HETATM  541 Y                 12.45712  15.15375  15.53898      Y   6 0
0.00000
HETATM  542 Zr                 9.99220  17.08495  16.08304      Zr  6 0
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HETATM  543 O                 11.61399  17.55280  17.20809      O   4 0
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HETATM  544 O                 15.93071  19.78465  15.53452      O   4 0
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HETATM  545 O                 14.71325  18.40388  19.42920      O   4 0
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HETATM  547 O                 14.45856  20.59887  17.79593      O   4 0
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HETATM  548 O                 12.05161  20.62122  17.16107      O   4 0
0.00000
HETATM  549 O                 14.51837  18.01806  16.73028      O   4 0
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HETATM  550 Zr                11.04371  19.19265  18.48614      Zr  6 0
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HETATM  551 Zr                13.41082  17.00713  18.33107      Zr  6 0
0.00000
HETATM  552 Zr                13.72141  19.75668  15.77642      Zr  6 0
0.00000
HETATM  553 Y                 15.68163   0.48273  -0.16664      Y   6 0
0.00000
HETATM  554 O                 17.39692   0.09136   1.14720      O   4 0
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HETATM  555 O                 16.16872   4.52871   3.91731      O   4 0
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HETATM  556 O                 19.42541   2.34605   3.84132      O   4 0
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HETATM  558 O                17.24269   2.26194   2.80398      O   4 0
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HETATM  559 O                19.21821   5.04768   3.34164      O   4 0
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HETATM  560 O                16.64212   4.61825   1.02467      O   4 0
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HETATM  561 O                19.85411   2.30464   1.36717      O   4 0
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HETATM  562 Zr               15.49267   3.44135   2.36480      Zr  6 0
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HETATM  563 Zr               18.66056   0.85527   2.59900      Zr  6 0
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HETATM  564 Y                18.13320   3.91457  -0.40699      Y   6 0
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HETATM  565 Zr               15.65981   6.25868   0.20854      Zr  6 0
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HETATM  566 O                17.23682   7.62066   1.15974      O   4 0
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HETATM  567 O                19.11129  10.33560   1.32752      O   4 0
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HETATM  568 O                19.78759   7.68176   3.47974      O   4 0
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HETATM  569 O                16.95086   9.79413   3.71915      O   3 1
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HETATM  570 O                19.55507  10.37752   3.71549      O   4 0
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HETATM  571 O                16.68404  10.13603   1.11149      O   4 0
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HETATM  572 O                19.73797   8.06974   0.70330      O   4 0
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HETATM  573 Zr               15.89898   8.62848   2.42092      Zr  6 0
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HETATM  574 Zr               18.48526   6.45020   2.02492      Zr  6 0
0.00000
HETATM  575 Zr               18.08260   9.12300  -0.21109      Zr  6 0
0.00000
HETATM  576 Y                15.58365   0.01368   5.03535      Y   6 0
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HETATM  577 O                17.01081   1.79181   6.45077      O   4 0
0.00000
HETATM  578 O                19.43670   4.47580   5.72517      O   4 0
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HETATM  579 O                19.68546   1.61435   8.08691      O   4 0
0.00000
HETATM  580 O                16.66800   6.57001   9.02467      O   3 1
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HETATM  581 O                17.07894   2.14142   9.12295      O   4 0
0.00000
HETATM  582 O                20.95215   6.41988   7.54630      O   4 0
0.00000
HETATM  583 O                16.83244   5.10579   6.56096      O   4 0
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HETATM  584 O                21.96091   1.85876   6.91609      O   4 0
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HETATM  586 Zr                17.89398   0.58777   7.73839      Zr  6 0
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HETATM  587 Y                 17.60378   3.31876   4.74074      Y   6 0
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HETATM  588 Zr                16.02533   6.53394   4.95671      Zr  6 0
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HETATM  589 O                 17.50962   7.66363   6.38850      O   4 0
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HETATM  590 O                 19.15995  10.12314   6.28304      O   4 0
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HETATM  591 O                 19.20766   4.54093   8.75829      O   4 0
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HETATM  592 O                 17.77079   9.97743   9.40714      O   3 1
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HETATM  593 O                 20.16688  10.67533   8.47487      O   4 0
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HETATM  594 O                 17.21752  10.04154   6.86197      O   4 0
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HETATM  595 O                 19.76107   7.48603   6.04346      O   4 0
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HETATM  596 Zr                16.84756   8.36951   8.29231      Zr  6 0
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HETATM  597 Zr                18.64412   6.14786   7.05902      Zr  6 0
0.00000
HETATM  598 Zr                18.51075   8.71872   4.84441      Zr  6 0
0.00000
HETATM  599 Y                 15.55566   0.10985  10.69157      Y   6 0
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HETATM  600 O                 16.93712   2.71140  12.28445      O   4 0
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HETATM  601 O                 20.95676   4.89279  11.25912      O   4 0
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HETATM  602 O                 18.98442   3.15246  13.84445      O   4 0
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HETATM  603 O                 16.65684   7.50497  13.95401      O   3 1
0.00000
HETATM  604 O                 16.28394   4.68906  14.63902      O   4 0
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HETATM  605 O                 19.58685   6.03790  13.75953      O   4 0
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HETATM  606 O                 16.83675   5.32513  11.95871      O   4 0
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HETATM  607 O                 19.32182   2.81887  11.64771      O   4 0
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HETATM  608 Zr                15.51688   4.08721  12.99058      Zr  6 0
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HETATM  609 Zr                18.35531   1.39252  12.97576      Zr  6 0
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HETATM  610 Y                 17.83252   3.93611  10.38850      Y   6 0
0.00000
HETATM  611 Zr                15.58825   6.82516  10.69649      Zr  6 0
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HETATM  612 O                 17.15540   8.38879  11.37524      O   4 0
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HETATM  616 O                18.96698  11.02276  14.59711      O   4 0
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HETATM  617 O                18.90108   7.38453   8.64238      O   4 0
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HETATM  618 O                18.92293   6.49728  10.74330      O   4 0
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HETATM  619 Zr               15.66767   9.07239  13.21469      Zr  6 0
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HETATM  620 Zr               18.21646   7.05709  12.70469      Zr  6 0
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HETATM  621 Zr               19.04611   8.81233  10.29393      Zr  6 0
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HETATM  622 Y                16.15361   1.06447  15.31723      Y   6 0
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HETATM  623 O                16.97408   2.59553  16.91073      O   4 0
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HETATM  624 O                20.17238   5.24757  16.66294      O   4 0
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HETATM  625 O                19.66775   2.87964  19.23928      O   4 0
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HETATM  626 O                16.79467   5.20875  18.97839      O   3 1
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HETATM  627 O                17.19677   2.49387  18.98130      O   4 0
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HETATM  630 O                19.38887   3.03686  16.86853      O   4 0
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HETATM  631 Zr               15.51962   3.59401  18.26240      Zr  6 0
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HETATM  632 Zr               18.50148   1.43716  17.79201      Zr  6 0
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HETATM  633 Y                18.21787   4.37861  15.59955      Y   6 0
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HETATM  634 Zr               15.54769   6.65477  15.57859      Zr  6 0
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HETATM  635 O                16.91089   8.52097  17.23413      O   4 0
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HETATM  639 O                19.33234  10.63585  19.56571      O   4 0
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HETATM  640 O                16.84946  10.26381  19.47416      O   4 0
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HETATM  643 Zr               17.95919   6.73559  18.19119      Zr  6 0
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HETATM  644 Zr               18.24475   9.70091  15.94111      Zr  6 0
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HETATM  645 Y                15.35393  11.40705  -0.01706      Y   6 0
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HETATM  646 O                16.77559  12.71309   1.26958      O   4 0
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HETATM  647 O                21.66638  15.92735   1.59729      O   4 0
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HETATM  648 O                19.19726  15.35830   1.87449      O   4 0
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HETATM  649 O                16.53287  15.21052   6.75634      O   3 1
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HETATM  650 O                17.26519  12.95975   3.88333      O   4 0
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HETATM  651 O                16.15328  15.10251   9.23671      O   4 0
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HETATM  652 O                16.82436  16.09654   1.27017      O   4 0
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HETATM  653 O                19.51342  12.73341   2.03148      O   4 0
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HETATM  654 Zr               15.44954  13.36681   2.88002      Zr  6 0
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HETATM  655 Zr               17.87052  11.52448   2.43359      Zr  6 0
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HETATM  656 Y                18.13727  14.57662  -0.00166      Y   6 0
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HETATM  657 Zr               15.85501  17.17868  -0.19916      Zr  6 0
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HETATM  658 O                16.97986  18.70541   1.25407      O   4 0
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HETATM  659 O                20.06767  20.38839   1.11725      O   4 0
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HETATM  660 O                19.51550  17.59719   3.77386      O   4 0
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HETATM  661 O                16.54787  18.50116   4.06859      O   3 1
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HETATM  662 O                19.85882  20.31377   3.55955      O   4 0
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HETATM  663 O                17.85903  21.01861   4.22403      O   4 0
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HETATM  664 O                19.69666  18.26098   1.26505      O   4 0
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HETATM  665 Zr               15.42490  18.81864   2.45269      Zr  6 0
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HETATM  666 Zr               18.21682  17.03116   2.45855      Zr  6 0
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HETATM  667 Zr               18.63176  19.48577   0.04588      Zr  6 0
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HETATM  668 Y                15.52290  10.46117   5.57901      Y   6 0
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HETATM  671 O                19.82571  12.63481   7.15929      O   4 0
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HETATM  672 O                14.58881  19.57175   9.25889      O   3 1
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HETATM  673 O                17.24901  12.74445   9.00919      O   4 0
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HETATM  674 O                19.07788  15.09491   7.22187      O   4 0
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HETATM  675 O                13.83386  14.58604   7.41747      O   4 0
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HETATM  676 O                22.41404  13.36912   6.60253      O   4 0
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HETATM  677 Zr               15.67843  13.62646   7.79217      Zr  6 0
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HETATM  678 Zr               18.20680  11.54590   7.91067      Zr  6 0
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HETATM  679 Y                18.08631  14.32993   5.28352      Y   6 0
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HETATM  680 Zr               15.41930  16.60240   4.84906      Zr  6 0
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HETATM  681 O                16.69131  17.92010   6.35421      O   4 0
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HETATM  682 O                24.09446  20.79783   6.24276      O   4 0
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HETATM  683 O                19.51419  17.31685   8.99950      O   4 0
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HETATM  684 O                17.32198  20.45288   9.43611      O   3 1
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HETATM  685 O                19.25241  20.33026   6.53467      O   4 0
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HETATM  686 O                16.61509  20.10919   6.82478      O   4 0
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HETATM  687 O                19.37105  17.49176   6.20864      O   4 0
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HETATM  688 Zr               15.17543  18.64992   7.53760      Zr  6 0
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HETATM  689 Zr               17.74555  16.64612   7.53506      Zr  6 0
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HETATM  690 Zr               18.31322  19.08330   4.87596      Zr  6 0
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HETATM  691 Y                15.57320  10.78048  10.88419      Y   6 0
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HETATM  692 O                17.07548  13.36517  11.83671      O   4 0
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HETATM  693 O                19.68441  15.91202  11.42256      O   4 0
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HETATM  694 O                19.75247  13.26374  14.26085      O   4 0
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HETATM  695 O                17.01380  18.42088  14.43072      O   3 1
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HETATM  697 O                19.96667  16.10831  13.82435      O   4 0
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HETATM  699 O                19.54445  13.33215  11.72274      O   4 0
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HETATM  700 Zr               15.69442  14.39579  13.14894      Zr  6 0
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HETATM  701 Zr               18.41639  12.21876  12.97457      Zr  6 0
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HETATM  702 Y                18.11857  14.55799  10.25812      Y   6 0
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HETATM  703 Zr               15.44100  16.73636  10.30522      Zr  6 0
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HETATM  704 O                16.84697  18.42685  11.75038      O   4 0
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HETATM  705 O                20.06839  21.01012  12.21043      O   4 0
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HETATM  706 O                19.67279  18.67101  14.26256      O   4 0
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HETATM  707 O                13.87075  21.60677  14.96482      O   3 1
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HETATM  708 O                18.66370  21.36953  14.77218      O   4 0
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HETATM  709 O                16.81664  20.87217  12.66494      O   4 0
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HETATM  710 O                19.65226  18.20696  11.55154      O   4 0
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HETATM  711 Zr               15.67942  19.26065  13.15949      Zr  6 0
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HETATM  712 Zr               18.31107  17.13088  12.99344      Zr  6 0
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HETATM  713 Zr               18.17791  18.58155  10.06347      Zr  6 0
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HETATM  714 Y                15.46114  11.58774  15.79499      Y   6 0
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HETATM  715 O                17.40935  11.58319  16.73154      O   4 0
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HETATM  716 O                19.49677  16.09283  16.79256      O   4 0
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HETATM  717 O                19.42624  13.50353  19.54542      O   4 0
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HETATM  718 O                17.07280  15.87986  19.39694      O   3 1
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HETATM  719 O                16.59258  13.13794  19.18483      O   4 0
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HETATM  720 O                19.63543  16.08697  19.93447      O   4 0
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HETATM  721 O                16.23075  15.28603  16.51547      O   4 0
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HETATM  722 O                19.15761  13.41717  17.52070      O   4 0
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HETATM  723 Zr               15.44208  14.43751  18.29040      Zr  6 0
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HETATM  724 Zr               18.22557  11.94579  18.62290      Zr  6 0
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HETATM  725 Y                18.07749  14.32114  15.78566      Y   6 0
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HETATM  726 Zr               15.82771  17.05729  15.52568      Zr  6 0
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HETATM  727 O                17.04795  17.72436  17.10363      O   4 0
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HETATM  728 O                20.45168  21.50128  17.54786      O   4 0
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HETATM  729 O                19.87586  18.39272  19.40918      O   4 0
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HETATM  730 O                17.30811  18.55246  19.67189      O   3 1
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HETATM  731 O                19.28098  21.14291  19.58062      O   4 0
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HETATM  732 O                17.41990  20.54324  17.53531      O   4 0
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HETATM  733 O                19.74215  19.27564  16.77451      O   4 0
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HETATM  734 Zr               15.93820  19.15268  17.88184      Zr  6 0
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HETATM  735 Zr               18.60843  17.08956  18.40875      Zr  6 0
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